

Self-adapting method for the localization of quantum critical points using Quantum Monte Carlo techniques

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 (February 1, 2008)

A generalization to the quantum case of a recently introduced algorithm (Y. Tomita and Y. Okabe, Phys. Rev. Lett. **86**, 572 (2001)) for the determination of the critical temperature of classical spin models is proposed. We describe a simple method to automatically locate critical points in (Quantum) Monte Carlo simulations. The algorithm assumes the existence of a finite correlation length in at least one of the two phases surrounding the quantum critical point. We illustrate these ideas on the example of the critical inter-chain coupling for which coupled antiferromagnetic $S = 1$ spin chains order at $T = 0$. Finite-size scaling relations are used to determine the exponents, $\nu = 0.72(2)$ and $\eta = 0.038(3)$ in agreement with previous estimates.

75.10.Jm, 75.40.Mg, 75.50.Ee, 02.70.Ss, 02.70.Tt

For studies of phenomena related to phase transitions, either classical or quantum, a precise determination of the critical point is of crucial importance, especially so in numerical work. For simulations of classical statistical models several algorithms [1,2] have been proposed, that automatically adjust to the critical point. Using ideas from invasion percolation Machta *et al.* [1] proposed an invaded cluster algorithm where critical clusters are generated directly, yielding the critical temperature as output. More recently, Tomita and Okabe [2] have suggested using a simpler method called probability-changing cluster algorithm to localize the transition temperature of Ising and Potts models within the framework of cluster algorithms. In Swendsen and Wang or Wolff algorithms [3], they propose to, *during* the simulation, either increase or decrease the probability p of connecting spins in the same cluster, and hence the temperature, according to whether the last clusters were percolating or not. Thus, systematically moving towards the cluster distribution at the critical point.

The generalization of either algorithm to the simulation of quantum systems would clearly be highly desirable but is difficult for several different reasons. Firstly, the structure of the clusters are more complicated than for classical systems and their relation to percolation physics is less clear. During the generation of a cluster it is not possible to assign a probability according to which a single “spin” is added to the cluster. Secondly, the dynamical critical exponent z , that links real and imaginary time correlations, is usually not known [4]. Hence, a direct generation of critical clusters would appear difficult due to the lack of knowledge of the relation between real-space and imaginary time correlations. A resolution of these difficulties would be very interesting and here we discuss a first step in this direction. We propose to generalize the approach of Tomita and Okabe [2] to Quantum Monte Carlo (QMC) simulations performed using

the loop algorithm [5]. We show that adjusting the critical parameter during the simulation according to whether an estimate of the correlation length is larger or smaller than some threshold, allows for a very precise determination of the quantum critical point. With relatively modest effort most of the associated critical exponents can also be determined.

The method we propose is closely related to the one suggested by Tomita and Okabe [2]. During the simulation a variable measuring the criticality of the system, in our case the correlation length ξ , is continuously monitored and one then changes a control parameter, λ , according whether or not this critical variable satisfies a criterion. Here λ can be the temperature $k_B T = 1/\beta$ as in Ref. [2] or directly a parameter of the Hamiltonian, controlling the transition. The algorithm should then equilibrate λ to an average critical value $\lambda_c(L)$, depending on the system size L , where the specified criterion is satisfied as an equality. The most difficult thing one has to do with this algorithm is to select a simple numerical criterion indicating whether the critical variable is in the ordered phase or not. As discussed in [2], by determining the critical value $\lambda_c(L)$ for different linear sizes L of systems, it is possible to obtain λ_c by extrapolating to the thermodynamic limit.

Let us briefly describe the method for a system of linear size L . First, one has to choose an initial value $\lambda_0(L)$ for the parameter λ . $\lambda_0(L)$ can be chosen according to a physical intuition of the critical point, or as the result of a very short preceding simulation at this size, or of the simulation for a shorter linear size. In most cases it is useful to choose $\lambda_0(L)$ to be in a phase with a finite correlation length. Then a certain number N_{warm} of “warmup” Monte Carlo steps are made to help the system to locate approximately $\lambda_c(L)$. During these steps, λ is modified by a certain amount $\pm \Delta_0 \lambda$ every N_t sweeps, according to our criterion which we will discuss later.

The N_t sweeps are needed to “thermalize” the system to the current value of λ to avoid autocorrelation problems (if λ is changed at every step, the configurations might be too correlated). Note that $\Delta_0\lambda$ is not necessarily fixed, and can for example be changed linearly from $\Delta_0\lambda$ to the smaller fixed value $\Delta\lambda$ used in the ensuing part of the calculation as discussed in [2]: this permits the system to take big steps in λ in the early stages of the simulation if $\lambda_0(L)$ is far from the critical value $\lambda_c(L)$. When the N_{warm} steps are finished, one makes N_{meas} steps of measurement with the same procedure : every N_t steps, λ is changed by a small and fixed value $\pm\Delta\lambda$ and estimates of observables (including λ) during the N_t steps are recorded. At the end of these N_{meas} sweeps, we get a distribution of λ centered around the critical value, $\lambda_c(L)$, for this system size. For the interpretation of the final distribution of λ it is important to have used a fixed value of $\Delta\lambda$ during the N_{meas} steps of measurement. We usually choose $\Delta\lambda \sim \frac{1}{V}$ where V is the volume of the system. Finally, in order to determine λ_c , the calculation is repeated for different linear sizes L and an extrapolation to the thermodynamic limit is performed, in principle allowing for a determination of the correlation length exponent ν . Other critical exponents can be determined in this step with the scaling of other observables.

Now we turn to a discussion of the criteria used to lower or raise λ . In Refs. [1,2] two criteria based on the percolation of the clusters were used. These criteria, which are referred to as the extension and topological rule in the related invasion cluster algorithm proposed by Machta *et al.* [1] for classical spin systems, can in principle also be used in QMC simulations with the loop algorithm: percolation or winding of loops can be used to determine the change in λ . However, the interpretation is in this case less clear. Most notably the exponential distribution of the size of the clusters is very wide and not very useful for a determination of λ_c . In particular, due to finite-size effects, it is not likely to change qualitatively when λ is tuned through the transition. Eventually, an algorithm based on the cluster distribution in the thermodynamic limit at $T = 0$ would be interesting to pursue, but the present method is in our opinion simpler and more general. Hence, we choose a different criterion: λ is modified according to an estimate of the correlation length ξ during the N_t steps. It is the same kind of criterion used in the fixed cluster algorithm [6]. It should be noted that this criterion is not necessarily related to the loops of the algorithm and can probably be used in other Monte Carlo simulations which do not admit a cluster algorithm. However, here the loop algorithm is very helpful because it quickly equilibrates configurations during the N_t sweeps and because it allows the use of improved estimators [7] for correlation lengths. Note the importance of using a reasonably large N_t to have a good estimate of the correlation length.

In the following, we will apply and check this method

to quantum $S = 1$ spin systems in order to determine the critical value of the perpendicular coupling, J^\perp , necessary for antiferromagnetic order at $T=0$ for coupled $S = 1$ spin chains. The $S = 1$ spin chain is known to be disordered [8] with a gap $\Delta_H \simeq 0.41J$ and a finite correlation length $\xi \simeq 6$ [9]. On the other hand, the $S = 1$ square antiferromagnet is Néel ordered at $T = 0$ [10] and it is known that a finite inter-chain coupling J_c^\perp , at which the system orders, exists [11–13]. We consider the following Hamiltonian:

$$H = \sum_{i=1}^L \sum_{j=1}^{L_y} [J \mathbf{S}_{i,j} \cdot \mathbf{S}_{i+1,j} + J^\perp \mathbf{S}_{i,j} \cdot \mathbf{S}_{i,j+1}], \quad (1)$$

with integer $S = 1$ spins and periodic boundary conditions. Previous work on this transition [11–13] has estimated the critical coupling and the exponents with the most recent estimate [13] for J_c^\perp being $J_c^\perp = 0.043648(8)$, a value surprisingly small compared to the Haldane gap $\Delta_H \simeq 0.41J$.

We investigate this quantum phase transition by setting our parameter λ as being the inter-chain coupling J^\perp . Our first criterion (A) is the following: if the calculated correlation length along the chains is larger than the system size ($\xi_x > L$), then the system is in an ordered phase for this value of J^\perp and we decrease J^\perp . If $\xi_x < L$, we increase J^\perp . The dividing criterion is thus:

$$\text{A} : \xi = L. \quad (2)$$

We then record the distribution of J^\perp , and estimate $J_c^\perp(L)$ for each lattice size. This criterion gives a good estimate of the value of the critical point, but will fail in determining it exactly and in determining critical exponents. This is due to the fact that an estimate of ξ for a system size where $\xi \simeq L$ suffers from pronounced finite-size effects. In particular, the extrapolation of $J_c^\perp(L)$ to the thermodynamic limit does not follow a simple scaling law allowing for a determination of the critical exponents. It is a well-known numerical fact that finite size corrections are significantly reduced when the lattice size is a few times larger than the calculated correlation length. Typically, if $6\xi < L$, finite-size corrections should be relatively unimportant. Hence, we use a second criterion (B)

$$\text{B} : \xi = \frac{L}{6}, \quad (3)$$

in order to reduce the finite-size corrections.

We use the continuous time QMC loop algorithm [5] where spins 1 are simulated by two symmetrized spins 1/2 [14] in the imaginary time direction. In order to study this quantum phase transition it is crucial to set $T \simeq 0$ and for this purpose we mainly use the recently proposed improvement of loop algorithm [15] which allows for simulations directly at $\beta = \infty$. Observables are

measured with the help of improved estimators [7]. In particular, the correlation length ξ is measured with the second moment method [16,7,14]. In general, simulations have been made on $L \times L_y$ lattices. For the smaller lattice sizes, square lattices were used with $T = 0$ [15]; for the largest lattice sizes $L_y < L$ (with $L_y \gg \xi_y$) was used and simulations were performed at a finite temperature significantly smaller than the smallest gap in the system. We typically set $N_t = 10^3$, $N_{\text{warm}} = 10^5$ and $N_{\text{meas}} = 10^6$ sweeps.

We now turn to a discussion of our results. In Fig. 1 we show an example of the distribution of J_c^\perp obtained during the simulation for $L = 66$ using criterion B. The

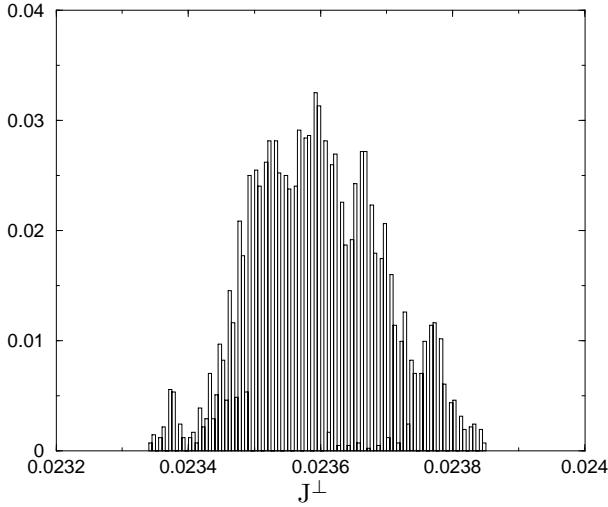


figure 1: Histogram of J_c^\perp obtained for the $L = 66, L_y = 10$ lattice at $T = 0$ with the criterion B ($\xi = \frac{L}{6}$). The distribution is peaked around $J_c^\perp(66) = 0.0236(1)$.

distribution is sharply peaked around a well defined mean value allowing for an easy determination of $J_c^\perp(L)$. In principle additional information pertaining to the critical exponents should be extractable from a detailed study of the scaling of the complete distribution with the system size L . For the simulations we have performed we did not have sufficient statistics to exploit this possibility. In Fig. 2 we show $J_c^\perp(L)$ as a function of L for the two criteria, A and B. As previously mentioned the criterion A suffers from pronounced finite-size effects. In particular, criterion A always *over estimates* the critical coupling. This might appear counter intuitive since the correlation length is expected to diverge at J_c^\perp . However, due to finite-size effects, the estimated correlation length never surpasses the linear size of the system until well inside the antiferromagnetic phase. One should note that for a finite quantum system there is always a finite gap restraining the correlation length. In order to extract the critical exponent we can as a first approximation fit the

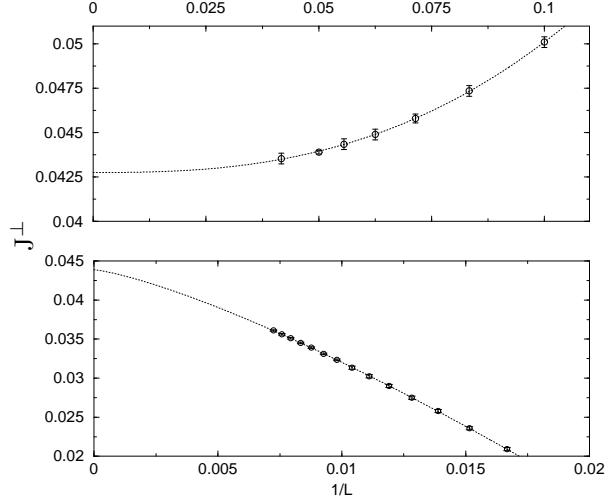


figure 2: $J_c^\perp(L)$ as a function of $1/L$ for the two different criteria A (top), B (bottom) used. Lines are fits to the equation (4) and give $J_c^\perp = 0.0428(4)$ for the criterion A and $J_c^\perp = 0.0438(4)$ for the B criterion. The values of $J_c^\perp(L)$ found for the first (second) criterion are always larger (smaller) than the critical coupling.

results obtained to a power law:

$$J_c^\perp(L) = J_c^\perp + AL^{-a}. \quad (4)$$

Here J_c^\perp is the critical coupling (in the thermodynamic limit) and A a constant. For the criterion B ($\xi_x = L/6$), $a = 1/\nu$ where ν is the correlation length exponent. For the criterion A, $a \neq 1/\nu$ due to finite-size corrections and the L dependence is non-trivial. We obtain $J_c^\perp = 0.0438(4)$ and $\nu = 0.77(2)$ for the criterion B, and $J_c^\perp = 0.0428(4)$ for the criterion A. The more reliable values are of course the first ones, but one can note that even with the criterion A, we have a good estimate of J_c^\perp . We can try to improve on this estimate by including corrections to scaling. In analogy with previous work on finite-size scaling [17] we include a first order finite-size correction to the correlation length.

$$\begin{aligned} \frac{L}{6} &= \xi - be^{-L/\xi} \\ \xi &= a(J_c^\perp - J_c^\perp(L))^{-\nu}. \end{aligned} \quad (5)$$

Including this finite size correction we find $\nu = 0.72(2)$, $J_c^\perp = 0.0436(2)$. In essence this correction amounts to a relatively precise estimate of the correlation length ξ in the thermodynamic limit for the given value of $J_c^\perp(L)$. This is then fitted to the expected form for the divergence of the correlation length as J_c^\perp is approached. In principle higher order corrections could be included, we have verified that in the present case they are extremely small. This value of J_c^\perp is in agreement with the recent QMC

“traditional” simulations [13] and is more precise than older results obtained with exact diagonalizations [11] or QMC [12] calculations.

Once a reliable estimate of $J_c^\perp(L)$ is obtained high-precision estimates of additional critical exponents can be obtained by performing calculations directly at $J_c^\perp(L)$. In Fig. 3 we show results

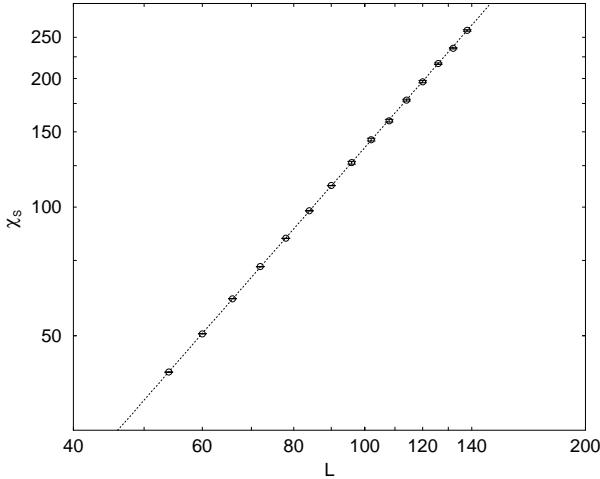


figure 3: The staggered susceptibility χ_s as a function of L on a log-log scale. The power-law fit (6) displayed as the line yields $\eta = 0.038(3)$.

of the size dependence (on log-log scale) of the staggered susceptibility χ_s with the criterion B ($\xi_x = L/6$). According to standard finite-size scaling theory this quantity should scale as

$$\chi_s(L) \sim L^{2-\eta}, \quad (6)$$

even with $J_c^\perp(L)$ a function of L . Additional finite size corrections of the form (5) for χ_s were not included. Fitting to this form (6), we obtain $\eta = 0.038(3)$ in complete agreement with previous estimates. The obtained values of η and ν for the critical exponents are in agreement with Matsumoto *et al.*’s results [13]. The exponents are very close to the values for the 3D classical Heisenberg model [18] confirming the expectation that two dimensional quantum phases transitions of quantum Heisenberg magnets belong to the university class of classical magnets [19] as seen in other simulations [20,13].

In this paper, we have proposed a very simple method to determine critical points in QMC simulations as a generalization of the probability-changing cluster algorithm [2] and applied it to determine the critical value of inter-chain coupling for spin $S = 1$ chains and calculate critical exponents for this quantum phase transition. The results are in agreement with previous estimates. It is important to underline that this method is easy to employ and adapt to other phase transitions and that it can

save a lot of computational effort. In particular, no a priori knowledge of z is needed. Most other methods, as for instance the use of Binder cumulants [21], would require the estimation of a critical quantity for many different system sizes for each value of the control parameter. The present method only requires the knowledge of the critical quantity for one system size for each of the control parameter. As mentioned in the introduction, it would be highly desirable to extend also the invaded cluster algorithm [1] to the simulation of quantum systems and we hope the present work could be a first step in that direction.

ACKNOWLEDGMENTS

We would like to thank S. Todo for valuable discussions and comments on the manuscript.

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